

HYDROGEN ATOM - COMPLETE WAVE FUNCTION

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.43.

If we combine all the results from the solution of the angular and radial equations for the hydrogen atom, we get a formula for the spatial wave function, which is given in Griffiths's book as eqn 4.89:

$$(0.1) \quad \psi_{nlm} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}} e^{-r/na} \left(\frac{2r}{na}\right)^l L_{n-l-1}^{2l+1} \left(\frac{2r}{na}\right) Y_l^m(\theta, \phi)$$

where L is an associated Laguerre polynomial and Y is a spherical harmonic.

The spherical harmonics can be calculated from a standard formula, as can the associated Laguerre polynomials. The forms of these functions vary according to the normalization. My version is

$$(0.2) \quad L_p^q(x) = c_0 \sum_{j=0}^p \frac{(-1)^j (p+q)!}{(p-j)!(q+j)!j!} x^j$$

The version in Griffiths sets $c_0 = (p+q)!$ (so it is that version that is used in the above formula for ψ_{nlm}) while some other sources use $c_0 = 1$.

For the spherical harmonics, the formulas are

$$(0.3) \quad Y_l^m(\theta, \phi) = \left[\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!} \right]^{1/2} e^{im\phi} P_l^m(\cos \theta)$$

with the P_l^m being the associated Legendre function:

$$(0.4) \quad P_l^m(x) = (1-x^2)^{m/2} \sum_{k=0}^{\lfloor (l-m)/2 \rfloor} \frac{(2l-2k)!}{2^l (l-k)! k! (l-2k-m)!} (-1)^k x^{l-m-2k}$$

As an example of using this formula, we'll construct ψ_{321} . We get $L_0^5(x) = 120$ and we worked out Y_2^1 in the previous post as

$$(0.5) \quad Y_2^1(\theta, \phi) = -\sqrt{\frac{15}{8\pi}} e^{i\phi} \sin \theta \cos \theta$$

Plugging these into the overall formula gives

$$(0.6) \quad \psi_{321} = -\sqrt{\left(\frac{2}{3a}\right)^3 \frac{1}{6 \times 120^3}} e^{-r/3a} \left(\frac{2r}{3a}\right)^2 (120) \left(\frac{15}{8\pi}\right)^{\frac{1}{2}} \sin \theta \cos \theta e^{i\phi}$$

$$(0.7) \quad = -\frac{1}{81\sqrt{\pi a^7}} r^2 e^{-r/3a} \sin \theta \cos \theta e^{i\phi}$$

To check the normalization, we do the integral:

$$(0.8) \quad \int_0^{2\pi} \int_0^\pi \int_0^\infty |\psi_{321}|^2 r^2 \sin \theta dr d\theta d\phi = \frac{1}{81^2 \pi a^7} \int_0^{2\pi} \int_0^\pi \int_0^\infty r^6 e^{-2r/3a} \sin^3 \theta \cos^2 \theta dr d\theta d\phi$$

$$(0.9) \quad = 1$$

using Maple for the integral.

The expectation value of r^s is (using Maple)

$$(0.10) \quad \langle r^s \rangle = \int_0^{2\pi} \int_0^\pi \int_0^\infty |\psi_{321}|^2 r^{2+s} \sin \theta dr d\theta d\phi$$

$$(0.11) \quad = \frac{1}{81^2 \pi a^7} \int_0^{2\pi} \int_0^\pi \int_0^\infty r^{6+s} e^{-2r/3a} \sin^3 \theta \cos^2 \theta dr d\theta d\phi$$

$$(0.12) \quad = \frac{1}{720} \left(\frac{3a}{2}\right)^s \Gamma(7+s)$$

The gamma function is infinite at all non-positive integral arguments, so this value is finite for $s > -7$ and all non-integer values less than -7 . The smallest integer value for which this is finite is $s = -6$. Note in particular that if $s = 0$, the formula reduces to $\langle r^0 \rangle = 1$ as it should.

The expectation value of r itself is

$$(0.13) \quad \langle r \rangle = \frac{21a}{2}$$

This is quite a bit bigger than the value for the ground state, which is $\langle r \rangle = 3a/2$.

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